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PDF MODELLING OF TURBULENT COMBUSTION

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SUMMARY

Important advances are being made in our understanding of turbulent combustion through the comparison between PDF model calculations and detailed experimental data. Previous calculations for the Sandia piloted jet flames have been extended in order to study the sensitivity to the pilot flame temperature and to radiative heat loss. Research is in progress on a new methodology ISAT-DR (*in situ* adaptive tabulation with dimension reduction) to incorporate detailed chemistry in turbulent combustion computations in an efficient manner. Both aspects of the work performed are advancing and demonstrating the capabilities of turbulent combustion modeling that can be applied to practical combustion devices.

PILOTED NONPREMIXED FLAMES

The piloted nonpremixed flames studied experimentally at Sandia (Barlow & Frank 1998) provide an excellent test of turbulent combustion models. These flames show distinct levels of interaction between turbulence and chemistry because of the increasing jet bulk velocities from flame D to F: flame D is close to equilibrium with a small amount of local extinction, whereas flame F is on the verge of global extinction. In each of these flames, the amount of local extinction reaches a peak at an axial distance of about 30 jet radii, with re-ignition occurring downstream. Several advanced approaches based on LES, CMC and PDF methods have been applied to compute these phenomena and have made significant progress. Notably, the joint PDF calculations of these flames by Xu and Pope (2000) and Lindstedt et al. (2000) show the best detailed agreement obtained between computations and the experimental data.

The PDF calculations of Xu & Pope (2000) and Tang et al. (2000) are capable of calculating, quantitatively, the observed phenomena of local extinction and reignition. These calculations are based on the modelled transport equation for the joint PDF of velocity, turbulence frequency, and composition. The sub-models of this method include the simplified Langevin model (SLM) for velocity and the Jayesh-Pope model (JPM) for turbulent frequency (see Pope 2000). The molecular mixing is modeled by the Euclidean minimal spanning tree (EMST) model of Subramaniam & Pope (1998), which features mixing locally in the composition space through interacting particles with neighboring particles. The reaction mechanism used is the 19 species, 15-step augmented reduced mechanism of Sung et al. (1998) which includes NO chemistry, and is denoted by ARM2. The chemical reaction calculations are performed using the *in situ* adaptive tabulation (ISAT) algorithm (Pope 1997). It should be pointed out that for each full-

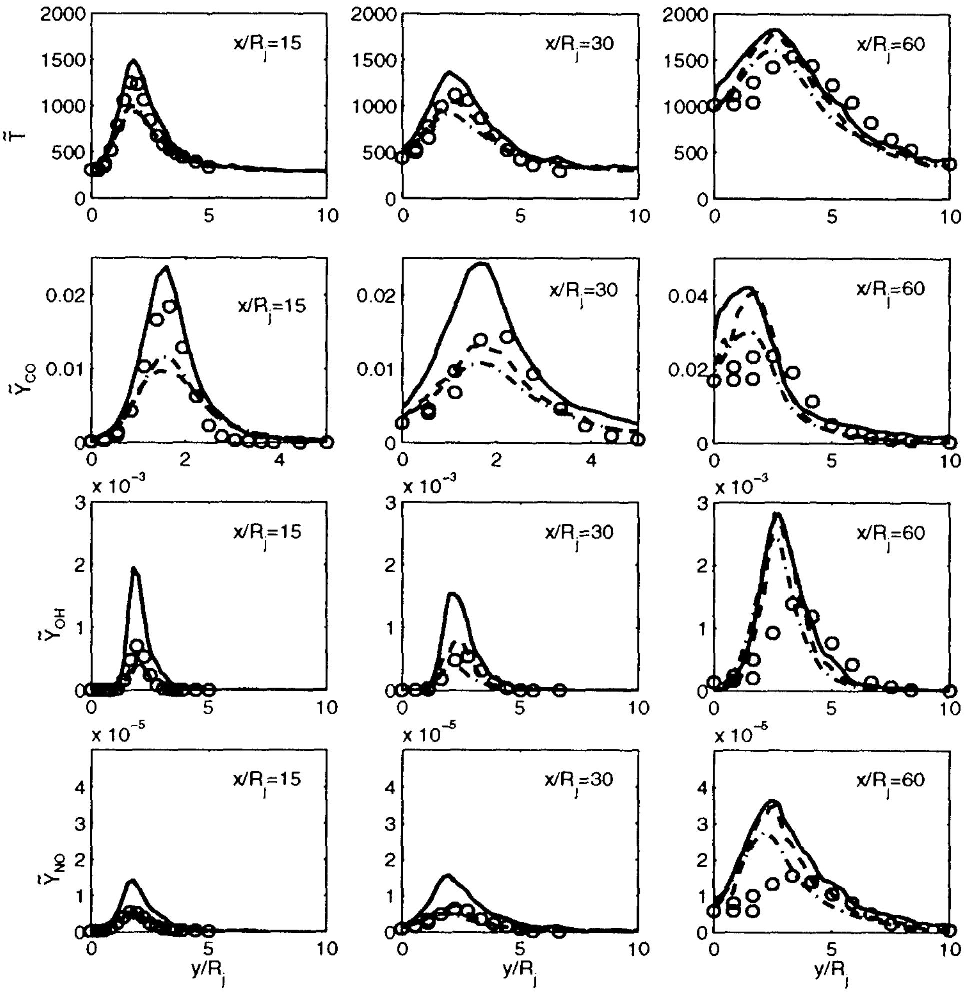

Fig. 1. Radial profiles of mean temperature and mass fractions in flame *F*: sensitivity to pilot temperature, T_p. Symbols, experimental data; solid line T_p = 1880K; dashed line T_p = 1870K; dot-dashed line T_p = 1860K.

scale PDF method calculation, the solution to the reaction equation system (20 dimensional) is required (of order) 10^9 times. ISAT can handle these computations economically and accurately. Recent work on PDF methods for these flames---now described---concerns sensitivity to the pilot flame temperature and to radiative heat loss.

It was observed by Xu & Pope (2000) that calculations of flame *F* exhibit some sensitivity to the pilot temperature T_p which is specified as a boundary condition. The experimental data show T_p in the range 1860K – 1880K, but the experimental accuracy may be no greater than 10-20K. This influence was studied systematically by performing calculations of flames *D* and *F* with pilot temperatures of T_p = 1860, 1870 and 1880K. For flame *D* it is found that the calculations are insensitive to T_p. But, as shown on Fig. 1, flame *F* exhibits extreme sensitivity. For example, at x/R_j = 15 and 30 the peak temperature decreases by about 500K and the mass fractions of *OH* decrease by a factor of more than two with a 10K decrease in pilot temperature. Similar trends exist for other variables. Particularly for *NO*, the results calculated using lower pilot temperatures give a perfect match with the experimental data at the first two locations shown in the figure. However, further downstream, all the modeled *NO* profiles overshot the peak value by a factor of more than two and do not predict correctly on the fuel rich side, although the temperature profiles seem to be satisfactory.

Figure 2 shows another manifestation of the sensitivity to the pilot temperature. The burning index (BI) is defined to be unity for complete combustion and zero for complete extinction. The figure shows substantially different results for T_p = 1860K and T_p = 1880K, with the experimental data generally falling between these two calculated values.

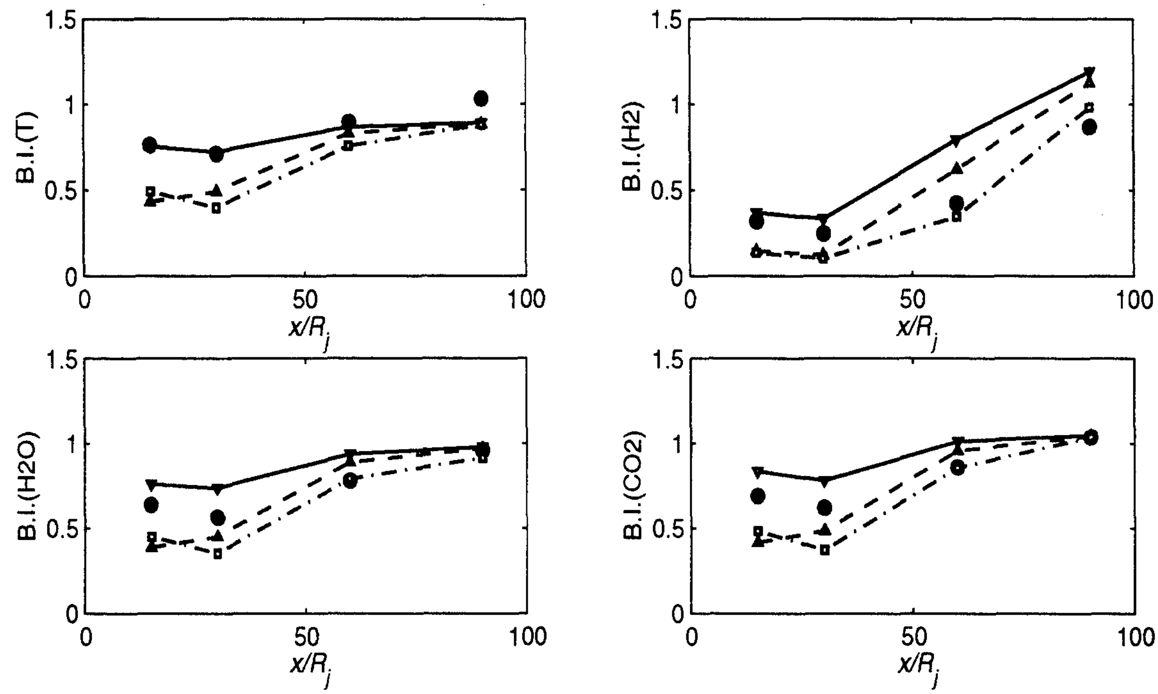

Fig. 2. Burning index (based on T and species) vs. axial distance in flame F. Symbols and lines as in Fig. 1.

The effects of radiative heat loss were investigated by performing "adiabatic" and "radiant" calculations. In the former all heat loss is neglected: in the latter, radiative heat loss is accounted for from the primary radiating species, CO_2, H_2O, CO and CH_4. We adopt an optically-thin limit radiation model, although the validity of this model for the 4.3-micron band of CO_2 is still in debate. Implemented in the framework of ISAT, the model includes the above four gas-phase emitting species with their Plank mean absorption coefficients calculated by RADCAL.

For flame D (not shown) the effect of radiation is to reduce the peak temperature by about 30K and to decrease the peak NO by 15%. Figure 3 presents the conditional mean profiles of four scalars, and shows completely different picture from the flame D results. For T_p = 1880K, the inclusion of radiation induces significant decreases in temperature and species mass fractions at the first three axial locations. The largest differences appear at x/R_j = 30 where the peak temperature decreases more than 500K and the species mass fractions decrease by a factor of two or three. This fact indicates that thermal radiation can significantly alter the local extinction status in this flame: not only is the NO chemistry strongly influenced by radiation, but also the reactions of other species such as OH and CO. The last column of Fig. 3 tells us that further downstream, the flame becomes closer to the equilibrium state as re-ignition takes place and the radiation tends to be less important.

Evidently, flame F is extremely sensitive to a decrease in temperature, whether it arises from T_p or from radiation.

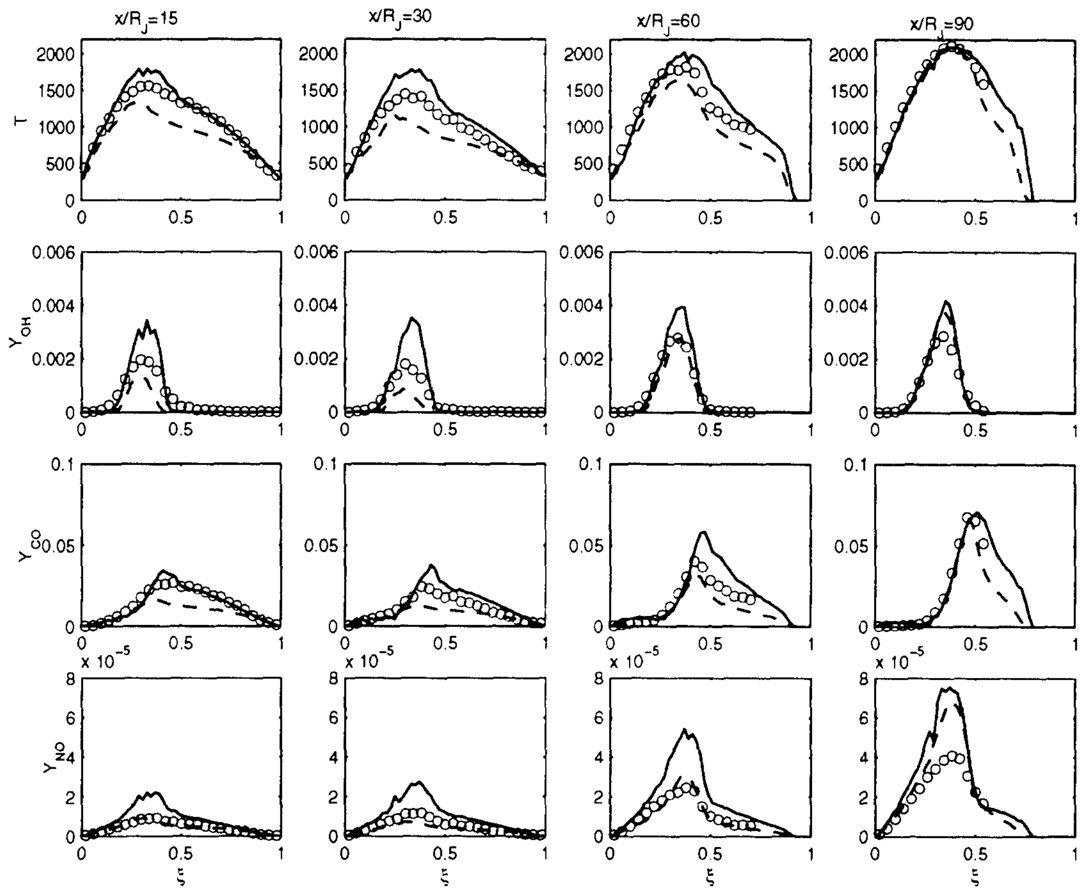

Fig. 3. Effect of radiative heat loss on means conditional on mixture fraction in flame *F*. Symbols, experimental data; solid line, adiabatic calculation; dashed line, radiant calculation.

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